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Distribution function of random strains in an elastically anisotropic continuum and defect strengths of T m3+ impurity ions in crystals with zircon structure

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Abstract

© 2017 American Physical Society. We construct a distribution function of the strain-tensor components induced by point defects in an elastically anisotropic continuum, which can be used to account quantitatively for many effects observed in different branches of condensed matter physics. Parameters of the derived six-dimensional generalized Lorentz distribution are expressed through the integrals computed over the array of strains. The distribution functions for the cubic diamond and elpasolite crystals and tetragonal crystals with the zircon and scheelite structures are presented. Our theoretical approach is supported by a successful modeling of specific line shapes of singlet-doublet transitions of the Tm3+ ions doped into ABO4 (A=Y, Lu; B=P, V) crystals with zircon structure, observed in high-resolution optical spectra. The values of the defect strengths of impurity Tm3+ ions in the oxygen surroundings, obtained as a result of this modeling, can be used in future studies of random strains in different rare-earth oxides.

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References

[1] G. A. Gehring, S. J. Swithenby, and M. R. Wells, Random strain fields on a molecular field system-dilute thulium vanadate, Solid State Comm. 18, 31 (1976). 10.1016/0038-1098(76)91394-6

[2] L. Savary and L. Balents, Disorder-Induced Quantum Spin Liquid in Spin Ice Pyrochlores, Phys. Rev. Lett. 118, 087203 (2017). 10.1103/PhysRevLett.118.087203

[3] J. -J. Wen, S. M. Koohpayeh, K. A. Ross, B. A. Trump, T. M. McQueen, K. Kimura, S. Nakatsuji, Y. Qiu, D. M. Pajerowski, J. R. D. Copley, and C. L. Broholm, Disordered Route to the Coulomb Quantum Spin Liquid: Random Transverse Fields on Spin Ice in (Equation presented), Phys. Rev. Lett. 118, 107206 (2017). 10.1103/PhysRevLett.118.107206

[4] S. Welinski, C. W. Thiel, J. Dajczgewand, A. Ferrier, R. L. Cone, R. M. Macfarlane, T. Chaneliere, A. Louchet-Chauvet, and P. Goldner, Effects of disorder on optical and electron spin linewidths in (Equation presented):(Equation presented), Opt. Mater. 63, 69 (2017). 10.1016/j.optmat.2016.09.039

[5] A. M. Stoneham, Shapes of inhomogeneously broadened resonance lines in solids, Rev. Mod. Phys. 41, 82 (1969). 10.1103/RevModPhys.41.82

[6] M. A. Ivanov, V. Y. Mirtofanov, L. D. Falkovskaya, and A. Y. Fishman, Random fields in disordered magnetics with Jahn-Teller ions, J. Magn. Magn. Mater. 36, 26 (1983). 10.1016/0304-8853(83)91040-5

[7] B. Z. Malkin, D. S. Pytalev, M. N. Popova, E. I. Baibekov, M. L. Falin, K. I. Gerasimov, and N. M. Khaidukov, Random lattice deformations in rare-earth-doped cubic hexafluoroelpasolites: High-resolution optical spectroscopy and theoretical studies, Phys. Rev. B. 86, 134110 (2012). 10.1103/PhysRevB.86.134110

[8] G. S. Shakurov, E. P. Chukalina, M. N. Popova, B. Z. Malkin, and A. M. Tkachuk, Random strain effects in optical and EPR spectra of electron-nuclear excitations in (Equation presented):(Equation presented) single crystals, Phys. Chem. Chem. Phys. 16, 24727 (2014). 10.1039/C4CP03437F

[9] F. Di. Trapani, X. Mateos, V. Petrov, A. Agnesi, U. Griebner, H. Zhang, J. Wang, and H. Yu, Continuous-wave laser performance of Tm:(Equation presented) under Ti:sapphire laser pumping, Laser Phys. 24, 035806 (2014). 10.1088/1054-660X/24/3/035806

[10] R. L. Melcher, E. Pytte, and B. A. Scott, Phonon Instabilities in (Equation presented), Phys. Rev. Lett. 31, 307 (1973). 10.1103/PhysRevLett.31.307

[11] J. D. Eshelby, The continuum theory of lattice defects, Solid State Phys. 3, 79 (1956). 10.1016/S0081-1947(08)60132-0

[12] I. M. Lifshitz and L. N. Rozentsveig, On the construction of the Green tensor for the fundamental equation of the theory of elasticity in the case of an unbounded elastically anisotropic medium, Zh. Eksper. Theor. Fiz. 17, 783 (1947) [in Russian].

[13] D. M. Barnett, The precise evaluation of derivatives of the anisotropic elastic Green's functions, Phys. Status Solidi B 49, 741 (1972). 10.1002/pssb.2220490238

[14] T. B. Biktagirov, A. N. Smirnov, V. Yu. Davydov, M. W. Doherty, A. Alkauskas, C. Gibson, and V. A. Soltamov, Strain broadening of the 1042-nm zero-phonon line of the NV-center in diamond: A promising spectroscopic tool for defect tomography, arXiv:1701.05631.

[15] S. A. Klimin, D. S. Pytalev, M. N. Popova, B. Z. Malkin, M. V. Vanyunin, and S. L. Korableva, High-resolution optical spectroscopy of (Equation presented) ions in (Equation presented): Crystal field energies, hyperfine and deformation splittings, and the isotopic structure, Phys. Rev. B 81, 045113 (2010). 10.1103/PhysRevB.81.045113

[16] H. J. McSkimin and P. Andreatch, Jr., The elastic moduli of diamond as a function of pressure and temperature, J. Appl. Phys. 43, 2944 (1972). 10.1063/1.1661636

[17] M. G. Brik, V. Krasnenko, and P. A. Tanner, Density functional studies of cubic elpasolites (Equation presented) ((Equation presented), Cl, Br) at ambient and elevated hydrostatic pressure, J. Lumin. 152, 49 (2014). 10.1016/j.jlumin.2013.10.070

[18] P. Mogilevsky, E. B. Zaretsky, T. A. Parthasarathy, and F. Meisenkothen, Composition, lattice parameters, and room temperature elastic constants of natural single crystal xenotime from Novo Horizonte, Phys. Chem. Minerals 33, 691 (2006). 10.1007/s00269-006-0118-6

[19] A. Armbruster, R. Thoma, and H. Werhle, Measurement of the elastic constants of (Equation presented) and (Equation presented) by Brillouin scattering and determination of Debye temperatures, Phys. Status Solidi A 24, K71 (1974). 10.1002/pssa.2210240154

[20] Z. Huang, L. Zhang, and W. Pan, Synthesis, structure, elastic properties, lattice dynamics and thermodynamics of (Equation presented) polymorphs from experiments and density functional theory calculation, J. Alloys Compounds 580, 544 (2013). 10.1016/j.jallcom.2013.07.031

[21] Z. Huang, L. Zhang, and W. Pan, Physical properties of zircon and scheelite lutetium orthovanadate: Experiment and first-principle calculation, J. Solid State Chem. 205, 97 (2013). 10.1016/j.jssc.2013.07.006

[22] P. Blanchfield and G. A. Saunders, The elastic constants and acoustic symmetry of (Equation presented), J. Phys. C. 12, 4673 (1979). 10.1088/0022-3719/12/22/010

[23] K. Hayasaka, R. Higashi, J. Suda, Y. Tanaka, S. Tamura, M. Giltrow, and J. K. Wigmore, Anomalous mode, elastic constants and phonon images in (Equation presented), Solid State Commun. 143, 386 (2007). 10.1016/j.ssc.2007.06.018

[24] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.96.014116 for the derivation of the strain distribution function, details of the crystal growth, lattice and elastic constants, crystal-field energies, and parameters of the electron-deformation interaction in (Equation presented)((Equation presented), Lu; (Equation presented), P) crystals.

[25] R. S. Feigelson, Flux growth of type (Equation presented) rare-earth vanadate crystals, J. Am. Ceram. Soc. 51, 538 (1968). 10.1111/j.1151-2916.1968.tb15689.x

[26] G. Garton, S. H. Smith, and B. M. Wanklyn, Crystal growth from the flux systems PbO-(Equation presented) and (Equation presented), J. Cryst. Growth 13-14, 588 (1972). 10.1016/0022-0248(72)90523-4

[27] R. S. Feigelson, Synthesis and single-crystal growth of rare-earth orthophosphates, J. Am. Ceram. Soc. 47, 257 (1964). 10.1111/j.1151-2916.1964.tb14409.x

[28] F. S. Ermeneux, C. Goutaudier, R. Moncorge, M. T. Cohen-Adad, M. Bettinelli, and E. Cavalli, Growth and fluorescence properties of (Equation presented)-doped (Equation presented) and (Equation presented) single crystals, Opt. Mater. 8, 83 (1997). 10.1016/S0925-3467(97)00029-3

[29] O. Guillot-Noel, Ph. Goldner, M. Bettinelli, and E. Cavalli, Electron paramagnetic resonance study of the multisite character of (Equation presented) ions in (Equation presented) single crystals, J. Phys.: Condens. Matter 17, 3061 (2005). 10.1088/0953-8984/17/19/019

[30] P. C. Becker, T. Hayhurst, G. Shalimoff, J. G. Conway, N. Edelstein, L. A. Boatner, and M. M. Abraham, Crystal field analysis of (Equation presented) and (Equation presented) in (Equation presented) and (Equation presented), J. Chem. Phys. 81, 2872 (1984). 10.1063/1.448060

[31] G. H. Fuller, Nuclear spins and moments, J. Phys. Chem. Ref. Data 5, 835 (1976). 10.1063/1.555544

[32] W. T. Carnall, G. L. Goodman, K. Rajnak, and R. S. Rana, A systematic analysis of the spectra of the lanthanides doped in single crystal (Equation presented), J. Chem. Phys. 90, 3443 (1989). 10.1063/1.455853

[33] K. D. Knoll, Absorption and fluorescence spectra of (Equation presented) in (Equation presented) and (Equation presented), Phys. Status Solidi B 45, 553 (1971). 10.1002/pssb.2220450218

[34] D. E. Wortman, R. P. Leavitt, and C. A. Morrison, Analysis of the ground configuration of (Equation presented) in (Equation presented), J. Phys. Chem. Solids 35, 591 (1974). 10.1016/S0022-3697(74)80014-4

[35] R. Lisiecki, P. Solarz, G. Dominiak-Dzik, W. Ryba-Romanowski, M. Sobczyk, P. Cherny, J. Sulc, H. Jelinkova, Y. Urata, and M. Higuchi, Comparative optical study of thulium-doped (Equation presented), and (Equation presented) single crystals, Phys. Rev. B 74, 035103 (2006). 10.1103/PhysRevB.74.035103

[36] C.-K. Loong, L. Soderholm, M. M. Abraham, L. A. Boatner, and N. M. Edelstein, Crystal-field excitations and magnetic properties of (Equation presented), J. Chem. Phys. 98, 4214 (1993). 10.1063/1.465028

[37] V. R. Pekurovskii, Calculations of thermodynamic characteristics of rare earth crystals with the zircon structure in the framework of microscopic theory, Izv. Akad. Nauk SSSR, Ser. Fiz. 50, 324 (1986) [in Russian].

[38] A. V. Vinokurov, A. M. Korovkin, B. Z. Malkin, V. R. Pekurovskii, A. I. Pominov, and A. L. Stolov, Piezospectroscopic studies of (Equation presented):(Equation presented) crystal, Fiz. Tverd. Tela 30, 2415 (1988)

[39] A. V. Vinokurov, A. M. Korovkin, B. Z. Malkin, V. R. Pekurovskii, A. I. Pominov, and A. L. Stolov [Sov. Phys. Solid State 30, 1392 (1988)].

[40] W. B. Mims, Phase memory in electron spin echoes, lattice relaxation effects in (Equation presented):Er, Ce, Mn, Phys. Rev. 168, 370 (1968). 10.1103/PhysRev.168.370

[41] R. D. Shannon, Revised effective ionic radii and systematic studies of interatomic distances in halides and chalcogenides, Acta Cryst. A 32, 751 (1976). 10.1107/S0567739476001551

[42] G. Davies, No phonon lineshapes and crystal strain fields in diamonds, J. Phys. C: Solid St. Phys. 3, 2474 (1970). 10.1088/0022-3719/3/12/014

[43] B. C. Chakoumakos, M. M. Abraham, and L. A. Boatner, Crystal structure refinements of zircon-type (Equation presented) ((Equation presented), Y, Ce, Pr, Nd, Tb, Ho, Er, Tm, Yb, Lu), J. Solid State Chem. 109, 197 (1994). 10.1006/jssc.1994.1091

[44] Y. Ni and J. M. Hughes, Crystal chemistry of the monazite and xenotime structures, Am. Miner. 80, 21 (1995). 10.2138/am-1995-1-203